

Users Manual For Double Spike GUI

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I. INTRODUCTION

This short document will overview the basic usage of the in-house double spike reduction program, as well as outline some of the extra calculations it is capable of performing. Additionally, this document will outline the format to prepare new elements and other files in order to expand the functionality of the program.

A. Mathematical Background of Double Spiking

In this section we outline the basic mathematical background of the double spike equations. For more information, please see CITE DOUBLE SPIKE TOOLBOX. The double spike equations are given by

$$\left\{ R_{S,i} \left(\frac{m_i}{m_{ref}} \right)^{-\alpha} \lambda + R_{T,i} (1 - \lambda) - R_{M,i} \left(\frac{m_i}{m_{ref}} \right)^{-\beta} = 0 \right\} \Big|_{i=1}^3 \quad (1)$$

where $R_{S,i}$ is the i^{th} isotope amount ratio of a known standard, $R_{T,i}$ is the i^{th} isotope amount ratio of your spike, $R_{M,i}$ is the i^{th} (measured) isotope amount ratio of a mixture of your sample and your spike T , m_i is the mass of the isotope in the numerator of your ratios R , m_{ref} is the mass of the reference isotope (that which appears in the denominator of your ratios), α is the natural fractionation factor, β is the fractionation factor of instrumental mass bias, and λ is a number related to the proportion of spike in your sample/spike mixture. The index i runs over the isotope amount ratios of your choice, however two must be ratios used in your enriched spike, and a third is the “reference” ratio used such that the above equations are exactly determined. In Equation 1 there are three unknowns: α , β , and λ . The set of equations in Equation 1 must be solved numerically, and to oversimplify, solving the above equation is all this program does.

Using the solutions to Equation 1, delta values can be calculated as

$$\delta^{\frac{N}{M}} X = \left[\left(\frac{m_N}{m_M} \right)^{-(\alpha_M - \alpha_{SM})} - 1 \right] \times 1000 \quad (2)$$

where X is the element of interest, m_N and m_M are the masses of the chosen isotopes, and α_{SM} comes from the solution of Equation 1 using the isotope amount ratios of a mixture of your known standard and spike for $R_{M,i}$. Based on the definition of Equation 2, it is important to note that Equation 1 is solved twice in order to calculate a delta value.

II. IMPORTANT FACTS ABOUT THE HOME SCREEN

The main menu and controller of the program is shown in FIG. 1. Below is some important information about this window.

1. The most important section is the “Column Headers” column, as these are the strings that the program will try to find in your data file. If the program cannot find a match to these strings in your data files, it will not be able to extract any data. Characters such as trailing spaces may have adverse effects for the programs ability to locate your desired data.
2. The “Mixture Ratio” is the measured (and hopefully calibrated) ratio of an appropriately prepared mixture of an international standard and your chosen double spike. Accurate measurement of this is important as these values define your $\delta = 0$ to which all your samples are compared.
3. The “Standard” column is the calibrated ratios of your international standard.
4. The “Spike Ratio” column is the measured ratio of your double spike

Column Headers	Mixture Ratio	Standard Ratio	Spike Ratio	Mass	Ratio Mass
92Mo/95Mo	4.66112	0.877076	147.091	91.90681	94.905841
94Mo/95Mo	0.584215	0.569169	1.1566	93.905841	
96Mo/95Mo	1.06347	1.068	0.855775	95.904678	
97Mo/95Mo	0.630014	0.623951	0.782161	96.90602	
98Mo/95Mo	4.25763	1.6078	93.4878	97.905407	
100Mo/95Mo	0.672026	0.665927	0.727959	99.907476	

Spike 1:

Spike 2:

Unspiked:

FIG. 1: This is the top menu of the program, not shown is the text box below where output will be produced.

5. The “Mass” column is the masses of the **numerator** of each of your ratios shown in the column headers column.
6. Finally, the “Ratio Mass” box is the mass of the isotope you’re using to calculate your ratios. For example, here, that is the mass of ⁹⁵Mo.
7. Each row is associated with its column header, for example in this file the 92Mo/95Mo ratio for each other column is in the first row. It is important that any custom files you prepare yourself follow this standard or else your calculations will be incorrect.
8. The Spike 1, Spike 2, and Spike 3 drop-down menus are what you use to choose which ratios to use in the double spike calculation.

If you’re working in terms of voltages, your main menu screen will look slightly different and appear as shown in FIG. 2

Column Headers	Mixture Ratio	Standard Ratio	Spike Ratio	Mass	Ratio Mass
92Mo	4.66112	0.877076	147.091	91.90681	94.905841
94Mo	0.584215	0.569169	1.1566	93.905841	
96Mo	1.06347	1.068	0.855775	95.904678	
97Mo	0.630014	0.623951	0.782161	96.90602	
98Mo	4.25763	1.6078	93.4878	97.905407	
100Mo	0.672026	0.665927	0.727959	99.907476	

Spike 1:

Spike 2:

Unspiked:

FIG. 2: The main window for use with files containing voltages instead of ratios

The only difference between the window with ratios shown in FIG. 1 and with voltages shown in FIG. 2 is the addition of the “Ratio Header” box. This is the column header of the voltage you’d like to use as the denominator in your calculations. The column headers section is also slightly different, as the headers in your file will be different. However, every other section is identical and it will be important to keep in mind that displayed constants will be in terms of the known **ratio** of those voltages.

Finally, it’s important to note that any value except column headers can be changed “on the fly” in the calculation by simply typing it in.

III. BASIC USAGE

A. Opening a Constants File

As the file containing the headers and constants controls the entire calculation, choosing the appropriate file is of the utmost importance. When you first open the program your first task will be to open an appropriate file in order to perform the double spike calculation. To do this, you must select **File** → **Open** → **Headers and Constants** → **<element_file_of_your_choice.py>**. Loading this file will control which options you have available to you for calculations. For example, if your column headers are given in terms of ratios, then performing a background subtraction will not be possible. If you've selected an appropriate file the window will update to show your new constants, and the text box will tell you the file you have chosen, as well if any interference files have been loaded along side it.

B. Choosing data to analyze

The program is capable of crawling through a directory and extracting data directly from Thermo ASCII grid exports from the Neptune software. However, if you want to manipulate your data off-line, it is also capable of opening CSV files. The CSV file format is explained in the next section. To open a directory for analysis simply click **File** → **Open** → **Directory** and simply choose the directory you've saved your ASCII grid exports in. The program will handle the rest. Alternatively, you can click **File** → **Open** → **CSV file** and open a CSV of data to analyze line-by-line instead.

C. How to format your CSV

NOTE: You cannot perform a background subtraction using CSV files from within this software.

Your CSV will need to be formatted much the same as the ASCII grid exports from the thermo software. The first column should be a list of sample name, and any columns after should be a list of the ratios or voltages you wish to analyse. Similar to below:

```
Name, ColumnHeader1, ColumnHeader2, ..., ColumnHeaderN
Sample, Data11, Data21, ..., DataN1
Sample2, Data12, Data22, ..., DataN2
...
...
...
SampleN, Data1N, Data2N, ..., DataNN
```

Where the program will read each line as an individual sample. You may need to modify your headers/constants file in order to accommodate your choice of column headers.

D. Calculation

Once you've selected a constant file and have opened a directory/CSV file, you simply need to choose your spike ratios/voltages and click calculate. This can be done by selecting the ratios of your choice from the drop down menus shown in FIG 1. If you do that, you'll see output similar to FIG. 3

From FIG. 3 we see the basic output of the program without any selections. The first output is the values for your standard and masses the program took from the main screen followed by a summary of values it was able to calculate. Currently, α , β and the percent spike as well as some options that we'll get to shortly are all that have been displayed. If you're interested in a delta value or concentrations, there are a few extra steps that you need to preform.

1. Calculating a Delta Value

In order to get a delta value you must select **Analysis Options** → **Choose Delta Value** where a window shown in FIG. 4 will pop up Using the window in FIG. 4, simply click your numerator and denominator mass and click done.

Used the following values for standard, mixture, spike, and mass:

	Standard	Mixture	Spike	Mass
92Mo/95Mo	0.877076	4.66112	147.091	91.90681
94Mo/95Mo	0.569169	0.584215	1.1566	93.905841
96Mo/95Mo	1.068	1.06347	0.855775	95.904678
97Mo/95Mo	0.623951	0.630014	0.782161	96.906602
98Mo/95Mo	1.6078	4.25763	93.4878	97.905407
100Mo/95Mo	0.665927	0.672026	0.727959	99.907476

Ratio Mass: 94.905841

Summary for Directory: /home/a10/Work/Code/Data/2013-Aug-21

File	Alpha	Beta	% Spike	Least Squares	Isobar Correction	Machine Fra
Sd0-1Micro.exp	1.57050319183	1.60917308938	50.8195891305	No	No	No
9-S2-49.exp	1.54928110777	1.61398743845	40.6724177348	No	No	No
36-1MicroFirst.exp	1.57259074057	1.66029291751	54.5337830768	No	No	No
12-S2-46.exp	1.5704917566	1.59889667848	39.4755766189	No	No	No
12-S2-75.exp	1.57207102432	1.61391846415	41.3923430835	No	No	No
9-S1-8.exp	1.55258525078	1.60551132788	38.6824546876	No	No	No
7-S2-93.exp	1.54227165924	1.63552321541	42.8486608952	No	No	No
11-S1-96.exp	1.56847470737	1.62553746767	41.6005551012	No	No	No
pkcl.exp	1.56516223912	1.67296177103	49.5736686207	No	No	No
8-S1-46.exp	1.53896167022	1.60461016601	43.3297221368	No	No	No
12-S2-54.exp	1.56556714631	1.5973518455	41.282631149	No	No	No
10-S1-7.exp	1.52781897743	1.59561560903	37.5808670013	No	No	No
11-S1-23.exp	1.41637894375	1.58001503796	49.6226823156	No	No	No
9-S1-86.exp	1.55283280703	1.60407836406	43.1652935957	No	No	No
39-Micro.exp	1.5398015718	1.61533384344	52.3058973231	No	No	No
11-S1-32.exp	1.37030959396	1.55144902004	52.7239953677	No	No	No
10-S1-98.exp	1.5420751519	1.57590641534	67.9419932132	No	No	No
12-S2-83.exp	1.56979264571	1.61014041918	40.5027367997	No	No	No
01-Micro.exp	2.1157435154	1.5057770527	00.7704155206	No	No	No

FIG. 3: The basic output of the program with no options selected

Choose Delta

Choose which masses to use in your delta value calculation.
These enter as (Mass1/Mass2)^(alpha_M - alpha_S)

Numerator mass	Denominator mass
<input checked="" type="radio"/> 92	<input checked="" type="radio"/> 92
<input type="radio"/> 94	<input type="radio"/> 94
<input type="radio"/> 95	<input type="radio"/> 95
<input type="radio"/> 96	<input type="radio"/> 96
<input type="radio"/> 97	<input type="radio"/> 97
<input type="radio"/> 98	<input type="radio"/> 98
<input type="radio"/> 100	<input type="radio"/> 100

Done

FIG. 4: The delta-value pop up selector

For example, to calculate $\delta_{95}^{98} Mo$ you would select 98 and 95.

Clicking **Calculate** again would return a delta value relative to your standard and mixture given from the main screen.

2. Concentration Calculation

To calculate concentrations by isotope dilution you must select **Analysis Options** → **Concentration Calculation** where the window shown in FIG. 5 will appear. In this window you will have to enter the concentration of your spike in whatever units you like, as well as the mass of spike added to each sample in whatever units you like. However, it's important to keep in mind that the units of concentration will be output in terms of

$$C_S = (\text{Unit of Spike Concentration}) \times (\text{Unit of Spike Mass Measurement})$$

File Name	Mass of spike added
SdO-1Micro.exp	0.0
9-S2-49.exp	0.0
36-1MicroFirst.exp	0.0
12-S2-46.exp	0.0
12-S2-75.exp	0.0
9-S1-8.exp	0.0
7-S2-93.exp	0.0
11-S1-96.exp	0.0
pkc1.exp	0.0
8-S1-46.exp	0.0
12-S2-54.exp	0.0
10-S1-7.exp	0.0
11-S1-23.exp	0.0
9-S1-86.exp	0.0
39-Micro.exp	0.0
11-S1-32.exp	0.0
10-S1-98.exp	0.0
12-S2-83.exp	0.0
Blank.exp	0.0
10-S1-32.5.exp	0.0

FIG. 5: The pop-up window to input concentrations

where C_S is the concentration of the sample. As an example if the concentration of your spike is given in nanograms per gram, and you measure the spike added in grams, the following is obtained:

$$C_S = \left(C_{spike} \left(\frac{\text{ng of Element}}{\text{g}} \right) \right) \times (M_{spike}(g)) = \text{ng of Element (in sample)}$$

where C and M are concentration and mass respectively. However, if input units of measurements are different, then a unit analysis will be required for every analysis to ensure correct concentrations.

Once that's all entered simply click **Finished** to commit these values to the calculation. If a box turns red, the program can't interpret your input as a number and you will need to fix it before continuing. Additionally **Refresh Values** simply sets all entries back to zero. At this point, by clicking **Calculate** your output should appear similar to FIG. 6.

There are a few important things to note about FIG 6 and other output that may be produced that is not seen in this screen shot:

- The masses used in the delta value calculation will always be printed at the top of the column
- Always scroll the window for additional information about the calculation performed.
- If each column reads **No Convergence** then the program was unable to solve the system. In this case try changing your reference ratio and repeating the calculation. If that doesn't work you have one remaining option: manipulate the data.

IV. VIEW

All that's in here is the ability to clear the text box from any extra stuff you don't want to look at anymore. If only you had such an option when marking assignments.

97Mo/95Mo	0.623951	0.630014	0.782161	96.90602		
98Mo/95Mo	1.6078	4.25763	93.4878	97.905407		
100Mo/95Mo	0.665927	0.672026	0.727959	99.907476		
Ratio Mass: 94.905841						
Summary for Directory: /home/a10/Work/Code/Data/2013-Aug-21						
File	Alpha	Beta	% Spike	Delta (98/95)	Concentration	Spike Added
Sd0-1Micro.exp	1.57050319183	1.60917308938	50.8195891305	0.424723943024	23.6657241323	24.0
9-S2-49.exp	1.54928110777	1.61398743845	40.6724177348	1.08558010103	0.0	0.0
36-1MicroFirst.exp	1.57259074057	1.66029291751	54.5337830768	0.359741202077	20.3878273929	24.0
12-S2-46.exp	1.5704917566	1.59889667848	39.4755766189	0.425079918807	37.4939359514	24.0
12-S2-75.exp	1.57207102432	1.61391846415	41.3923430835	0.375918914078	34.6246068666	24.0
9-S1-8.exp	1.55258525078	1.60551132788	38.6824546876	0.982660330633	38.7725471875	24.0
7-S2-93.exp	1.54227165924	1.63552321541	42.8486608952	1.30395037128	32.6285189536	24.0
11-S1-96.exp	1.56847470737	1.62553746767	41.6005551012	0.487872132083	34.3304199843	24.0
pkc1.exp	1.56516223912	1.67296177103	49.5736686207	0.591000234309	24.8767338015	24.0
8-S1-46.exp	1.53896167022	1.60461016601	43.3297221368	1.40708533973	31.9959620604	24.0
12-S2-54.exp	1.56556714631	1.5973518455	41.282631149	0.578393562955	34.78436824	24.0
10-S1-7.exp	1.52781897743	1.59561560903	37.5808670013	1.75435528656	40.6383164695	24.0
11-S1-23.exp	1.41637894375	1.58001503796	49.6226823156	5.23409507504	24.8732053184	24.0
9-S1-86.exp	1.55283280703	1.60407836406	43.1652935957	0.974949700626	32.2055862588	24.0
39-Micro.exp	1.5398015718	1.61533384344	52.3058973231	1.38091408931	22.3066992433	24.0
11-S1-32.exp	1.37030959396	1.55144902004	52.7239953677	6.6761496836	21.9813894164	24.0
10-S1-98.exp	1.5420751519	1.57590641534	67.9419932132	1.31007298879	11.542701849	24.0
12-S2-83.exp	1.56979264571	1.61014041918	40.5027367997	0.446843304471	35.9232128755	24.0
Blank.exp	2.11575435154	1.59597720627	99.7794165206	-16.405625185	0.0537087810475	24.0
10-S1-32.5.exp	1.55252322396	1.58696097614	40.9238036461	0.984592288211	35.3094098841	24.0

FIG. 6: Note that the other options seen previously have still been printed, you will simply have to scroll the bottom text bar in order to see if any additional parameters have been selected.

V. ADVANCED ANALYSIS OPTIONS

In this section the other options that may appear under the **Analysis Options** tab are explored. Note that this menu can become a separate window by clicking the dashed line. This proves convenient for repeated analysis.

A. Least Squares Solve

By selecting this option you no longer solve Equation 1 exactly as a three-equation system. In this case the program will look for least squares solutions using

$$\left\{ R_{S,i} \left(\frac{m_i}{m_{ref}} \right)^{-\alpha} \lambda + R_{T,i} (1 - \lambda) - R_{M,i} \left(\frac{m_i}{m_{ref}} \right)^{-\beta} = 0 \right\} \Bigg|_{i=1}^N \quad (3)$$

where N is the number of ratios. In this case, the program finds the optimum α, β and λ that minimizes the residual of the error between all equations. This solution may produce “unsatisfactory” results as compared to the three equation system. However, these solutions should be more exact for a chemically-pure sample, or after appropriate background subtraction and interference corrections have been applied.

B. Interference Correction

NOTE: Both these corrections work with Least-Squares

NOTE: This option only appears if you have an interference file associated with your constants/headers.

NOTE: If you’re working with ratios you *cannot* correct for isobaric interferences in the denominator of your ratio.

By selecting this option, if your header file has been associated with an appropriate interference file, the program will subtract isobaric interferences from your sample ratios using a measured isobar provided in your ASCII grid export. This function applies the following correction to your data:

$$\left\{ R_{i,Corrected} = R_{i,Measured} - I_{i,Measured} \times \frac{(\text{Abundance of Isobaric Interference})_i}{\text{Abundance of } I_{measured}} \right\} \Bigg|_{i=1}^N \quad (4)$$

where $R_{measured}$ is your measured ratio, and $I_{measured}$ is the measured ratio of your interference. In this case the numerator mass in $R_{corrected}$ is the same mass as that of the interference abundance.

If you're working with voltages, the program applies the following correction:

$$\left\{ V_{i,Corrected} = V_{i,Measured} - I_{i,V\ Measured} \times \frac{(\text{Abundance of Isobaric Interference})_i}{\text{Abundance of } I_{V\ measured}} \right\}_{i=1}^N \quad (5)$$

where $V_{Corrected}$ is the corrected voltage, $V_{Measured}$ is the measured voltage, and $I_{V\ Measured}$ is the voltage of the isobaric interference. The calculation regarding voltages is identical with the exception that you are now free to apply isobaric corrections to your chosen denominator in the ratio as well.

C. Machine Fractionate Interference

NOTE: This works with least squares solutions

NOTE: This option only appears if you have an interference file associated with your constants/headers.

NOTE: This is an untested and experimental correction, use it with caution.

NOTE: This option is only implemented when using ratios. Voltage files won't work. So don't try (You probably won't be able to).

By selecting this option the program will attempt to get a better estimate of a true isobaric interference by machine fractionating the interference file. This requires us to solve the system twice. First we solve the system using the correction in Equation 4. Then, using the β term from the solution to Equation 1 or 3, the measured data set is then corrected by

$$\left\{ R_{i,Corrected} = R_{i,Measured} - I_{i,Measured} \times \frac{(\text{Abundance of Isobaric Interference})_i}{\text{Abundance of } I_{measured}} \times \left(\frac{M_{i,I}}{M_{ref}} \right)^{-(\beta_M - \beta_{SM})} \right\}_{i=1}^N \quad (6)$$

where M_I is the mass of the interference isobar, M_{ref} is the mass of your reference mass, β_M is the machine fractionation calculated from using a standard/spike mixture, and β_{SM} is the machine fractionation calculated from the measured sample, and i runs over the chosen ratios. The system is then solved again with the corrected interferences subtracted.

This allegedly provides a better estimate of the actual isobaric interferences, but again, this is untested and I recommend you test it before publish any data using it.

D. Subtract Background

NOTE: This works with least squares solutions

NOTE: This option only appears if you're using a voltage based constant/header file.

This option is on by default. By selecting this flag the program will prompt you to select a background file (typically a measurement of 3% HNO_3) from which the program will subtract those measurements from each sample like

$$\{V_{i,corrected} = V_{i,measured} - V_{i,HNO_3}\}_{i=1}^N \quad (7)$$

where this correction is applied to all voltages.

E. Separate Background File

This applies the same correction as above, but allows you to choose a separate background file for each sample. The window that opens is asking you to choose a file which contains your measurement of 3% HNO_3 to subtract from the filename given at the top of the window. If there is no filename displayed, simply resize the window until it appears.

VI. THE NEW TAB

Under this tab is the tools required in order to create new header and constant files, as well as isobaric interference files.

A. Headers and Constants

By clicking **New** → **Headers and Constants**, the following window shown in FIG 7 will open.

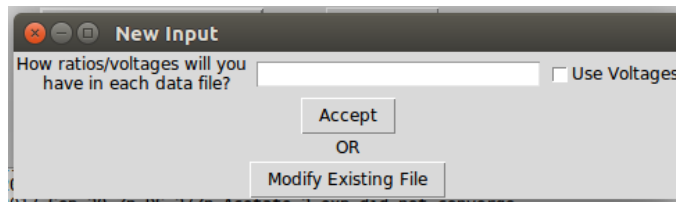


FIG. 7:

You are presented with two options. By selecting **Modify Existing File** you will be prompted to open an existing header file, and you will be free to edit it to your liking and save a new file (or overwrite the existing one) with your changes made. If you need to make a header file for a new element/simply to start fresh, you must first enter how many ratios you will require in your header file. If your element has 10 isotopes, in principle you may want to type 9 here in order to have information about each ratio. Generally speaking you will enter $N - 1$ here where N is the number of isotopes. By selecting the **Use Voltages** button, you will be able to prepare a file which uses voltages instead of ratios. You will still need to enter $N - 1$ in the entry box. Once you click accept, you will be presented with a window that is similar to FIG 8.

NOTE: You can only have a maximum of 12 rows.

Column Headers	Mixture Ratio	Standard Ratio	Spike Ratio	Mass	Ratio Mass
					Ratio Header

FIG. 8:

In FIG. 8 you will have to fill this menu completely. Under the column headers you must enter a string or value that represents the header of each column of interest. Additionally you must enter the numerical ratios of **Mixture Ratio** or the ratio of whatever isotope in the associated row and your chosen ratio (either one you've chosen explicitly in ratio-based calculations, or the isotope specified under **Ratio Header**). The **Standard Ratio** is the ratios of your standard, **Spike Ratio** is the ratios of your spike, **Mass** is the mass of each isotope in the numerator of the ratio, and **Ratio Mass** is the mass of the isotope in the denominator of your ratio, and in the case of voltage-based files, you'll also need to enter the column header of your chosen ratio isotope under the **Ratio Header** section. When you're finished click **Create Input File** and save your new file where ever you'd like. Once it's saved, simply load it and it's ready to use.

NOTE: If any entry boxes turn red, you have entered a non-numerical value where you should only have numbers, or left a column header blank.

IMPORTANT: If you have two ratios in your THERMO file that are identical but you have perhaps applied a correction to one, your header needs to include the column number in the thermo file. For example, if you have something like 96Mo/97Mo (1) and 96Mo/97Mo (8) in your THERMO file, but your column header is only 96Mo/95Mo, the program will only find 96Mo/97Mo (8). If you need the first column, you need to have 96Mo/97Mo (1) entered into your header/constant file. However, you can enter both in the same file provided you don't want to use least squares solutions to prevent tedious file switching. If you do this, DO NOT mix and match ratio and voltage headers in the same file if you want your results to make sense.

B. Interference Correction

In order to correct for isobaric interferences you must first create an file of isotopic abundance information about the isobar. To do this, click **New** → **Interference Correction** you will first be prompted to select a constants/header

file. The file you select is the headers/constants file that the correction will be associated with. If you want to apply an isobaric correction, you must create this file for each set of headers/constants. Once you select an appropriate file, a window similar to FIG. 9 will appear

FIG. 9: Shown here is an example for Zinc

In the window shown in FIG 9, you will need to enter some information. Below is an outline of the information you will be required to enter

1. **Measured Isobar Header.** This column header needs to appear in your THERMO exports, and it needs to be that of an isotope that doesn't appear in your analysis elements (eg. if you're measuring molybdenum and you want to correct for zirconium interferences, measure ^{91}Zr not ^{92}Zr). It is this string that the program will look for in order to subtract the scaled voltage/ratio from the ratios with isobars.
2. **NOTE:** If you're working with ratios, you **MUST** measure that isobar with a common denominator to your files.
3. **Abundance of Measured Isobar.** This is where you need to enter the elemental abundance of the isotope that you've measured. For example, if your isobar is 50% abundant, enter 0.5. Finally you are required to enter the mass of this isobar under **Mass of Measured Isobar**.
4. **Columns of interest in chosen data file:**, to the right of these are the headers from the constant/header file you chose. These labels are important. If you have an isobaric interference on the **NUMERATOR** of your ratio, or the voltage, below each header label you are required to enter the abundance of your isobaric interference, and the mass of that isobaric interference.
5. **Abundance of Isobar.** The elemental abundance of the isobaric interference on the numerator/voltage of the column header in your THERMO file.
6. **Mass of Isobar.** The mass of the isobaric interference.
7. **NOTE:** You cannot correct for isobaric corrections on the denominator if you only measured ratios.
8. If you click **New Isobar** you can correct for additional measured isobaric interferences, however, this functionality is untested and I can't guarantee it will work. Once you've entered your isobaric interferences, hit accept and save your file anywhere you'd like.
9. **NOTE:** If you do not have an isobaric interference on a mass for a given element, leave that entry blank.

C. Data Base Entry

By selecting this you will commit the results of the last calculation you did to the lab database. I think this works for all data, but I didn't have much to test it with so I don't guarantee this will work every time. But if it does, you'll be prompted for the pass word (which isn't in this document) and if it's correct that data should get into the database. You will still have to enter all other information using the **DataBaseEntry** program.

VII. SAVING YOUR ANALYSIS

To save your analysis, select **File** → **Save** → **Output**. You will be prompted to enter a file name and location to save a file. This will save the entire contents of the programs output to your specified file.

VIII. BASIC TROUBLE SHOOTING. OR: IT'S NOT MY FAULT; IT'S YOURS

A. Could not find headers error

If the program outputs an error message similar to this:

```
File <your_file>.exp did not contain all your chosen column headers.
Found: None None None
where 'None' indicates missing data
```

The first possibility that you've selected the wrong element for the data sets you're trying to analyze. Change the constants file to one appropriate for your data. If the header file is for the element in your directory, there are two possibilities:

1. Your column headers have been modified (for example, with iron the label for ^{56}Fe changes every run as you have to recenter off the Ar peak). Open your data file and double check that you have entered the correct headers.
2. Sometimes the desired column headers in your constants file may look identical to the ones in your ASCII grid exports and you'll still get this message. In this case modify your constant file headers by copy/pasting the headers directly from your data files followed by saving and loading your modified file. This should fix the problem. This is caused by the program looking for the *exact* match to the headers you've entered, and a direct copy paste is the best course of action. Don't enter spaces either.

B. I've selected a headers and constant file but none of the values or buttons appear

This happens when the program opens certain python files that aren't formatted correctly for the program to use. In this case, simply open a file that is formatted correctly and it should solve the problem.

C. Program doesn't seem to be grabbing correct numbers

If you have multiple columns with identical headers, the program will extract data from only the LAST item it finds. If you are applying corrections from within the THERMO software to the same ratio/voltage, be sure to change the column header for each instance to ensure that the program can locate all data you hope to run through this program. The THERMO software will put a (#) tag after each ratio, and if you want to look at any changes caused by corrections applied by the THERMO software then you'll have to include the (#) tags in your column headers.

D. I want it to do something not mentioned in this manual

It can't .